now, $\underline{H = H_0 + V}$ vs $\underline{H_0}$

$$\Rightarrow \quad \mathcal{G}(z) = \frac{1}{z - H_0 - V} \quad \text{vs} \quad \mathcal{G}_0(z) = \frac{1}{z - H_0}.$$

By using the identity, $\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$

$$= \frac{1}{A} + \frac{1}{A-B} B \frac{1}{A}$$

$$\Rightarrow \quad \underline{\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}} \ ! \qquad // \ A \equiv z - H_0, \quad B \equiv V$$

$$\hookrightarrow \mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 + \mathcal{G}_0 V \mathcal{G}_0 V \mathcal{G}_0 + \cdots$$

... Born series"

$\Rightarrow$ Integral equation for the Green's function.

$$G(\vec{x}, \vec{x}') = G_0(\vec{x}, \vec{x}') + \int d\vec{s}\; G_0(\vec{x}, \vec{s})\, V(\vec{s})\, G(\vec{s}, \vec{x}')$$

// E is omitted.

(5) The Feynman Path Integral."

Dirac: $\exp\left[\frac{i}{\hbar} \underbrace{\int_{t_1}^{t_2} dt\, L_{\text{classical}}}_{= S \text{ (classical action)}}\right]$ corresponds to $\langle x_2 t_2 | x_1 t_1 \rangle$.

???

Feynman: $\exp\left[\frac{i}{\hbar} S\right]$ is proportional to $\langle x_2 t_2 | x_1 t_1 \rangle$. !

path integral

$$\Rightarrow \quad \langle x_N t_N | x_1 t_1 \rangle = \int_{x_1}^{x_N} \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}.$$

- A single free particle in 1D (t-indep.)

$$H = \frac{\tilde{p}^2}{2m} + V(\tilde{x},\cancel{t}) \equiv T(\tilde{p}) + V(\tilde{x})$$

- We want to compute

$$K(b,a) = \langle x_b | \mathcal{U}(t_b,t_a) | x_a \rangle \, \Theta(t_b - t_a)$$

$$\equiv (x_b t_b) \qquad \equiv (x_a t_a)$$

- Recipes of the path integral representation :

① breaking the evolution from a to b into a large sequence of κ small forward steps in time of duration τ by means of the composition property for $\mathcal{U}$;

② evaluating each small step explicitly;

③ Showing that these steps sum to the form $\sum_P e^{\frac{i}{\hbar}S}$, where S is the classical action for some path P composed of linear segment from a to b;

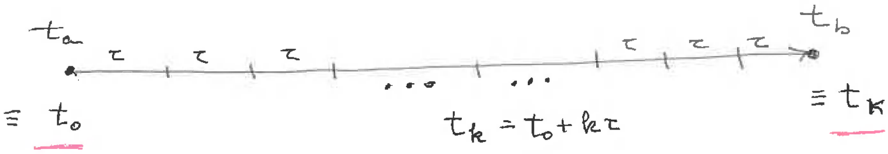
(④ Taking the limit, $\tau \to 0$, $\kappa \to \infty$, $\kappa\tau = t_b - t_a$.)

We assume this from the beginning!

→ Now, let's compute $K(b,a)$.

- <u>Step 1</u> : Break it into pieces.

$$K(b,a) = \langle x_b | \mathcal{U}(t_b, t_b - \tau) \cdots \mathcal{U}(t_a + 2\tau, t_a + \tau)\, \mathcal{U}(t_a + \tau, t_a) | x_a \rangle$$



NOTE : $K \equiv N$, $\tau = \Delta t$ in Sakurai.

$$k = 0, 1, \cdots, \frac{t_b - t_a}{\tau}$$

Let $x_a \equiv x_0$, $x_b \equiv x_K$ as well.

$$\Rightarrow K(b,a) = \int_{-\infty}^{\infty} dx_{N-1} \cdots dx_1 \, \langle x_N | e^{-\frac{i}{\hbar}H\tau} | x_{N-1} \rangle \cdots$$

$$\cdots \langle x_2 | \underbrace{e^{-\frac{i}{\hbar}H\tau}}_{\text{a propagator } \langle x_2 t_2 | x_1 t_1 \rangle} | x_1 \rangle \langle x_1 | e^{-\frac{i}{\hbar}H\tau} | x_0 \rangle .$$

= (a product of propagators) "

- Step 2: compute $\langle x_{k+1} t_{k+1} | x_k t_k \rangle$ by using that τ is small "

  (This is also hard because of "V").

  - ~~A~~ naive thought

$$e^{-iH\tau/\hbar} \simeq 1 - \frac{i}{\hbar}H\tau \longrightarrow \text{a big error} .$$

[a composition property breaks down in $O(\tau^2)$.]

  - The Better one : the Suzuki-Trotter decomposition "

$$e^{-\frac{i}{\hbar}H\tau} \simeq e^{-\frac{i}{\hbar}T\tau} \, e^{-\frac{i}{\hbar}V\tau} \quad \text{when } \tau \text{ is small.}$$

$\longrightarrow$ perfect unitarity!

‖ NOTE : Baker-Campbell-Hausdoff (BCH) theorem.

$$e^A e^B = \exp\left(A + B + \frac{1}{2}[A,B] + \frac{1}{12}\left([A,[A,B]] - [B,[A,B]]\right) \cdots \right)$$

$$\Rightarrow \langle x_{k+1} | e^{-\frac{i}{\hbar}H\tau} | x_k \rangle \simeq \underbrace{\langle x_{k+1} | e^{-\frac{i}{\hbar}T\tau} | x_k \rangle}_{\text{a free-particle propagator}} e^{-\frac{i}{\hbar}V(x_k)\tau}$$

$$= \sqrt{\frac{m}{2\pi i\hbar\tau}} \exp\left[\frac{i}{\hbar} \left(\frac{m(x_{k+1} - x_k)^2}{2\tau} - \tau V(x_k) \right) \right] .$$

Step 3: It's done.

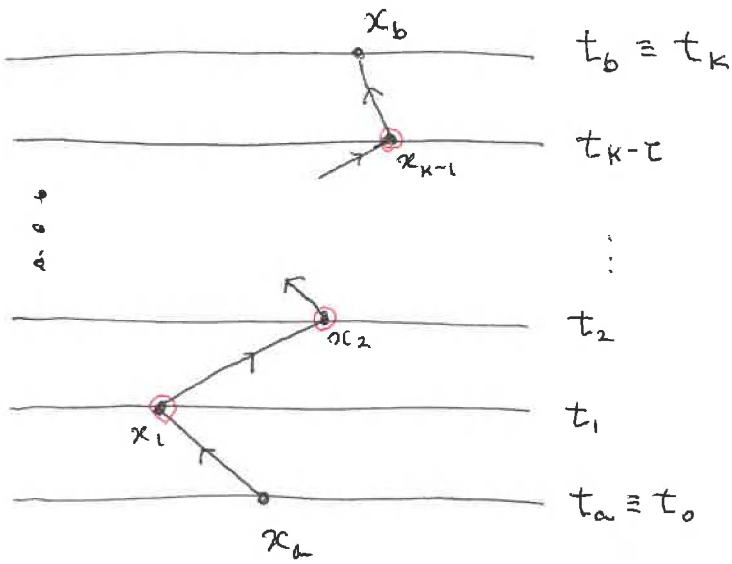
$$K(b,a) = \lim_{\substack{\tau\to 0 \\ K\to\infty \\ (\,K\tau = t_b - t_a\,)}} \left(\frac{m}{2\pi i \hbar \tau}\right)^{\frac{1}{2}K} \int_{-\infty}^{\infty} dx_{K-1}\cdots dx_1 \,\cdot$$

$$\cdot\, \exp\left[\frac{i\tau}{\hbar}\sum_{k=0}^{K-1}\left(\frac{m}{2\tau^2}(x_{k+1}-x_k)^2 - V(x_k)\right)\right].$$

→ It can be evaluated by using PIMC.
(path-integral Monte Carlo.)

- Meaning and a shorter form.

Integrand : a "path". $\int\cdots\int =$ sum over the paths.



☆ The beads ◎ move freely, but feel the adjacent beads.

☆ The links ↗ are just like springs!

$\left(\frac{m}{2\tau^2}(x_{k+1}-x_k)^2\right)$: a harmonic term!

One can also see

$$\lim_{\tau\to 0}\left(\frac{m}{2\tau^2}(x_{k+1}-x_k)^2 - V(x_k)\right) = \frac{1}{2}m\dot{x}_k^2 - V(x_k)$$

$$= L_{\text{classical}}(x_k, \dot{x}_k; t_k).$$

NOTE:

$$\frac{dx}{dt} = \lim_{\Delta t\to 0}\frac{\Delta x}{\Delta t}$$

So it's classical!

$$\Rightarrow \lim_{\substack{\tau\to 0\\ K\to\infty\\ K\tau = t_b - t_a}} \tau \sum_{k=0}^{K-1} L_{\text{classical}}(x_k, \dot{x}_k ; t_k) = \int_{t_a}^{t_b} dt\, L(x,\dot{x};t)$$

$$= S_{ba}[x(t)] \leftarrow \text{Classical Action "for } x(t)\text{"} ☆$$

$$\Rightarrow K(b,a) = \int_a^b \mathcal{D}[x(t)] \exp\left(\frac{i}{\hbar} S[x(t)]\right).$$

$$\| \quad \int_a^b \mathcal{D}[x(t)] \equiv \lim_{(\cdots)} \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dx_{K-1}\cdots dx_1$$

(b) Free-particle Path Integral (as an example.)

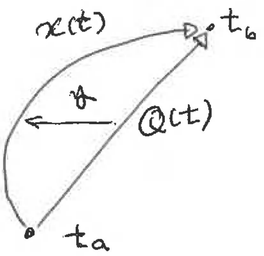
$$K(b,a) = \lim_{\tau\to 0} \left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dx_{K-1}\cdots dx_1 \exp\left[\frac{i\tau}{\hbar}\sum_{k=0}^{K-1} m \frac{(x_{k+1}-x_k)^2}{2\tau^2}\right].$$

: Some trouble occurs at fixed beads – x_0, x_K.

→ Let's substract the classical "path" from $x(t)$.

$\equiv Q(t)$: fixed

→ devations $y(t) = x(t) - Q(t)$



$$\Rightarrow \sum_{k=0}^{K-1} (x_{k+1}-x_k)^2 = \sum_{k=0}^{K-1} (Q_{k+1}-Q_k)^2 + \sum_{k=0}^{K-1} (y_{k+1}-y_k)^2 + \cancel{2\sum_{k=0}^{K-1} \underbrace{(Q_{k+1}-Q_k)}_{=\text{const.}}(y_{k+1}-y_k)} \to 0$$

const. (velocity = const.)

$\because \sum \Delta y = 0$

$$\Rightarrow S[x(t)] = \frac{m}{2}\int_{t_a}^{t_b} dt \left[\dot{Q}^2(t) + \dot{y}^2(t)\right]$$

and $\displaystyle\int_{t_a}^{t_b} dt\, \frac{1}{2} m \dot{Q}^2(t) = \frac{1}{2} m \left(\frac{x_b - x_a}{t_b - t_a}\right)^2 \cdot (t_b - t_a) = \frac{1}{2} m \frac{(x_b-x_a)^2}{t_b - t_a}$

$\equiv S_{cl}(b,a) \leftarrow$ along classical "path"

$$\Rightarrow K(b,a) = \int_a^b \mathcal{D}[x(t)]\, e^{\frac{i}{\hbar} S[x(t)]}$$

$$= F(t_b - t_a) \cdot e^{\frac{i}{\hbar} S_{cl}(b,a)}$$

where $$\underbrace{F(t_b - t_a)}_{\text{time translation invariant}} = \int_{t_a}^{t_b} \mathcal{D}[y(t)]\, e^{\frac{i}{\hbar}\int_{t_a}^{t_b} dt\, \frac{1}{2} m \dot{y}^2(t)}$$

(free particle!)

$\parallel$ $y(t_a) = y(t_b) = 0$.

- Evaluation of $F(t)$ $\parallel$ $t_a = 0$, $t_b - t_a \equiv t$.

① quick and easy, but specific. $\parallel$ (y, t') : a way point.

$$F(t) = \int_{-\infty}^{\infty} dy\, K(0,t\,;\,y,t')\, K(y,t'\,;\,0,0)$$

$\Leftarrow$ composition property is used.

$(x=0,\ t=0) \xrightarrow{\quad F \quad} (x=0,\ t=t)$

$(x=y,\ t')$

$$= \int_{-\infty}^{\infty} dy\, F(t-t')\, e^{\frac{i}{\hbar}\frac{y^2}{t-t'}\cdot\frac{m}{2}}\, F(t')\, e^{\frac{i}{\hbar}\frac{y^2}{t'}\cdot\frac{m}{2}}$$

$$= F(t-t')\, F(t') \int_{-\infty}^{\infty} dy\, \exp\left[i y^2 \left(\frac{1}{t-t'} + \frac{1}{t'} \right) \frac{m}{2\hbar} \right]$$

$$= F(t-t')\, F(t') \sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t'(t-t')/t}\,.$$

$\hookrightarrow$ factored as :

$$\left(\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t}\, F(t) \right) = \left[\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t-t'}\, F(t-t') \right] \left[\sqrt{\frac{2\pi i\hbar}{m}} \sqrt{t'}\, F(t') \right].$$

$$\therefore\ F(t) = \sqrt{\frac{m}{2\pi i\hbar t}} \Rightarrow \underbrace{K(b,a) = \sqrt{\frac{m}{2\pi i\hbar (t_b - t_a)}}\, e^{\frac{i m (x_b - x_a)^2}{2\hbar (t_b - t_a)}}}_{\text{as expected...}}$$

③ Elaborative but general.

$$F(t) = \lim_{\tau\to 0}\left(\frac{m}{2\pi i\hbar\tau}\right)^{\frac{K}{2}} \int_{-\infty}^{\infty} dy_{K-1}\cdots dy_1 \exp\left[\frac{i}{\hbar}\cdot\frac{1}{2}m\sum_{k=0}^{K-1}\frac{(y_{k+1}-y_k)^2}{\tau}\right]$$

→ change of variables : $\eta_k = y_k\sqrt{\frac{m}{\hbar\tau}}$

$$\Rightarrow F(t) = \lim_{\tau\to 0}\left(\frac{m}{\hbar\tau}\right)^{\frac{1}{2}}\cdot\left(\frac{1}{2\pi i}\right)^{\frac{K}{2}}\int_{-\infty} d\eta_{K-1}\cdots d\eta_1\, e^{\frac{i}{2}\sum_{k=0}^{K-1}(\eta_{k+1}-\eta_k)^2}$$

: This is just a multidimensional Gaussian integral.

$$* \int d^n x\, e^{-\frac{1}{2}\vec{x}^T A\vec{x}} = \sqrt{\frac{(2\pi)^n}{\det[A]}}$$

Use the identity,

$$\sum_{k=0}^{K-1}(\eta_{k+1}-\eta_k)^2 = \vec{\eta}^T\cdot A\cdot\vec{\eta} \quad \Big\| \quad \vec{\eta}^T = (\eta_1,\cdots\eta_k\cdots,\eta_{K-1})$$

$$\Big\| \quad \eta_0 = \eta_K = 0.$$

where $A = \begin{pmatrix} 2 & -1 & 0 & \cdots \\ -1 & 2 & -1 & \cdots \\ 0 & -1 & 2 & -1 \\ \vdots & & -1 & 2 & -1 \\ & & & \ddots & \ddots \end{pmatrix}$ "Laplacian matrix"

($K-1$ by $K-1$ matrix)

→ easy to diagonalize : $A = U\tilde{\lambda}U^\dagger$
↳ eigenvalues.

→ change of variables $\vec{\xi} = U^\dagger\vec{\eta}$

$$\Rightarrow F(t) = \lim_{\tau\to 0}\sqrt{\frac{m}{2\pi i\hbar\tau}}\prod_{k=1}^{K-1}\int_{-\infty}^{\infty}\frac{d\xi_k}{\sqrt{2\pi i}}e^{\frac{i}{2}\lambda_k\xi_k^2} \qquad \begin{aligned}&\vec{\eta}^T A\vec{\eta} = \vec{\xi}^T\tilde{\lambda}\vec{\xi}\\ &\Big\| \; = \sum_k \lambda_k\xi_k^2\end{aligned}$$

$$= \lim_{\tau\to 0.}\sqrt{\frac{m}{2\pi i\hbar\tau\prod_{k=1}^{K-1}\lambda_k}}$$

$\therefore$

$$F(t) = \lim_{\substack{\tau\to 0\\ K\to\infty\\ \|\,\tau K = t}}\sqrt{\frac{m}{2\pi i\hbar\tau\det[A]}} \qquad \Big\| \quad \text{and we know that } \det[A] = K$$

↳ reproduces $K(b,a)$